

**Free Vibration and Bending Analysis of Uniformly
Distributed Carbon Nanotube Composite Plate Using
Finite Element Method**

Ajay Kumar Paswan

Free Vibration and Bending Analysis of Uniformly Distributed Carbon Nanotube Composite Plate Using Finite Element Method

Thesis Submitted to

National Institute of Technology, Rourkela

*for the award of the degree
of*

Master of Technology

In Mechanical Engineering with Specialization

“Machine Design and Analysis”

by

Ajay Kumar Paswan

Roll No. 213me1383

Under the Supervision of

Prof. Subrata Kumar Panda



**Department of Mechanical Engineering
National Institute of Technology Rourkela
Odisha (India) -769 008**

May- 2015



NATIONAL INSTITUTE OF TECHNOLOGY
ROURKELA
CERTIFICATE

This is to certify that the work in this thesis entitled “**Free Vibration and Bending Analysis of Uniformly Distributed Carbon Nanotube Composite Plate Using Finite Element Method**” by **Mr. Ajay Kumar Paswan** (213ME1383) has been carried out under my supervision in partial fulfilment of the requirements for the degree of **Master of Technology** in Mechanical Engineering with **Machine Design and Analysis** specialization during session 2013 - 2015 in the Department of Mechanical Engineering, National Institute of Technology, Rourkela.

To the best of my knowledge, this work has not been submitted to any other University/Institute for the award of any degree or diploma.

Date:

Prof. S. K. Panda
(Assistant Professor)
Dept. of Mechanical Engineering
National Institute of Technology
Rourkela-769008

SELF DECLARATION

I, Mr Ajay Kumar Paswan, Roll No. 213ME1383, student of M. Tech (2013-15), Machine Design and Analysis at Department of Mechanical Engineering, National Institute of Technology Rourkela do hereby declare that I have not adopted any kind of unfair means and carried out the research work reported in this thesis work ethically to the best of my knowledge. If adoption of any kind of unfair means is found in this thesis work at a later stage, then appropriate action can be taken against me including withdrawal of this thesis work.

NIT Rourkela
25 may 2015

Ajay Kumar Paswan

ACKNOWLEDGEMENT

My first thanks are to the Almighty God, without whose blessings, I wouldn't have been writing this “acknowledgments”. I am extremely fortunate to be involved in an exciting and challenging research project work on “**Free Vibration and Bending Analysis of Uniformly distributed Carbon Nanotube Composite Plate Using Finite Element Method**”. It has enriched my life, giving me an opportunity to work in a new environment of ANSYS and LAMMPS. This project increased my thinking and understanding capability as I started the project from scratch.

I would like to express my greatest gratitude to my supervisor **Prof. S. K. Panda**, for his excellent guidance, valuable suggestions and endless support. He has not only been a wonderful supervisor but also an honest person. I consider myself extremely lucky to be able to work under guidance of such a dynamic personality. He is one of such genuine person for whom my words will not be enough to express.

I would like to express my sincere thanks to **Vishesh R. Kar, Vijay K. Singh and P.V. Katariya, Kulmani Mehar** (My seniors) and all my classmates for their precious suggestions and encouragement to perform the project work. I am very much thankful to them for giving their valuable time for me.

Finally, I express my sincere gratitude to my parents for their constant encouragement and support at all phases of my life.

Ajay Kumar Paswan

Abstract

In this work, free vibration and bending behaviour of uniformly distributed carbon nanotube composite plate are analysed. The material properties of single-walled carbon nanotube evaluated through molecular dynamics simulation using LAMMPS software. The effective material properties of the composite plates are obtained using an extended rule of mixture. A finite element model is developed for the single-walled carbon nanotube composite plate using ANSYS Parametric Design Language (APDL) code in ANSYS environment. For the discretization purpose, an eight-noded serendipity shell element is used from the ANSYS library. Subsequently, the validation study is performed through the available published literature. Finally, the parametric study is demonstrated by varying different material and geometrical parameters for free vibration and bending responses of composite plate.

Keywords: Carbon Nanotubes, Composite plate, Molecular Dynamics, FEM, ANSYS.

Contents

Title Page		(I)
Certificate of Approval		(III)
Self-Declaration		(IV)
Acknowledgement		(V)
Abstract		(VI)
Contents		(VII)
List of Symbols		(XI)
List of Tables		(XIV)
List of Figures		(XV)
Chapter 1	Introduction	1-7
1.1	Overview	1-2
1.2	Types of CNTs	2-4
1.3	CNTs geometry	4-5
1.4	Applications of CNTs	5-6
1.5	Motivation of the Current Work	6 -7
1.6	Aim and Scope of the Present Thesis	7
Chapter 2	Literature Review	9-13
Chapter 3	General Mathematical Formulation	13-33

3.1	Molecular dynamics simulation	13-23
3.1.1	Structure of carbon nanotube	16-17
3.1.2	Force fields and total potential energy	17-23
3.2	Finite Element Method and ANSYS	18-23
3.3	Carbon nanotube composite plate.	24-26
3.4	Free vibration of CNT composite plate.	26-28
3.5	Bending analysis of CNT composite plate.	28-30
Chapter 4	Results and Discussion	31-40
4.1	Types of Carbon nanotube and Volume fraction validation.	31
4.2	Evaluation of material properties of carbon nanotubes.	32
4.3	Numerical illustrations of bending analysis.	33
4.4	Numerical illustrations of free vibration analysis.	36
Chapter 5	Conclusions	41
	Future Scope of the Research	42
	References	43-47

List of Symbols

Record of the symbols is defined as they occur in the thesis. Some of most common symbols, which are used repeatedly, are listed below:

x_l, y_l, z_l	Co-ordinate axis of plane
E_1, E_2 and E_3	Young's modulus
G_{12}, G_{23} and G_{13}	Shear modulus
ν_{12}, ν_{23} and ν_{13}	Poisson's ratios
a, b and h	Length, width and thickness of the plate
$\{\epsilon_i\}$	Linear strain directions
$\{\sigma\}$	Stress direction at mid-plane
$\{\delta\}$	Displacement vector
$[K_s]$	Spring constant of bonding stretching
$[K_\theta]$	Force constant of bending
$[K_\phi]$	Force constant of torsion
F	Force on each atom
$U_{S.E.}$	Strain energy

U	Potential energy
Φ_0	Ideal phase
V_0	Initial volume of CNTs
a_{c-c}	Length of carbon atom
$r_i \text{ and } r_j$	Position vector
$[T]$	Function of thickness co-ordinate
α	Thermal expansion co-efficient
ρ	Density of the material
T	Kinetic energy
a/h	Thickness ratio
R/a	Curvature ratio
E_1/E_2	Modular ratio

Abbreviation

APDL	ANSYS parametric design language
SSSS	All edges simply supported
CCCC	All edges clamped
HHHH	All edges hinged
LAMMPS	Large-scale atomic molecular massively parallel simulation

VMD	Visualisation molecular dynamics
Eq.	Equation
GPa	Giga Pascal
MPa	Mega pascal
Nm	Nano mete

List of Tables

Table No		Page No.
1	The comparison of non-dimensional elastic modulus for different volume fraction.	31
2	The comparison of material properties in molecular dynamics.	32
3	The material properties of (10, 10) SWCNT.	33
4	The non-dimensional central deflection for different thickness ratio (a/h) validation using volume fraction. (SSSS).	34
5	The non-dimensional central deflection for different thickness ratio (a/h) using volume fraction. (a) CCCC.	35
6	The non-dimensional central deflection for different thickness ratio (a/h) using volume fraction. (b) SCSC.	36
7	The non-dimensional fundamental frequency for different thickness ratio validation using volume fraction. (SSSS).	37
8	The non-dimensional fundamental frequency for different thickness ratio using volume fraction. (a) CCCC.	38
9	The non-dimensional fundamental frequency for different thickness ratio using volume fraction. (b) SCSC.	39

List of Figures

Figure No.		Page No.
1	Volume fraction of reinforcement (fiber)	2
2	Types of carbon nanotube.	4
3	Arrangement of carbon nanotubes (CNTs) for armchair, zig-zag and chiral.	5
4	Interatomic interaction in molecular dynamics notion.	14
5	Boundary loading conditions for SWCNT armchair (10,10).	15
6	The graphite plane of nanotube surface coordinates.	16
7	Solid and Hollow CNTs through MD.	23
8	Shell 281 element description.	25
9	Carbon nanotube reinforced composites plate.	28
10	Variation of elastic modulus for different types of fibres	32
11	The effect of thickness ratio on non-dimensional central deflection(SSSS).	34
12	The effect of thickness ratio on non-dimensional central deflection.(CCCC)	35
13	The effect of thickness ratio on non-dimensional central deflection. (SCSC)	36
14	The effect of thickness ratio on non-dimensional fundamental frequency.(SSSS)	37
15	The effect of thickness ratio on non-dimensional fundamental frequency.(CCCC)	38
16	The effect of thickness ratio on non-dimensional fundamental frequency.(SCSC)	39

CHAPTER 1

INTRODUCTION

1.1 Overview

Composite materials are defined as a group of two or more materials on a macroscopic scale. These are always used because of its some unique properties like stiffness, strength, light weight, corrosion resistance, thermal properties, and wear resistance. Composites have two constituent elements namely, reinforcement (fibre) and matrix. The fibres are used in modern composites because of its high specific mechanical properties compared to those of old-style bulk materials. The reinforcement (fibre) is categorised as continuous fibre, short fibre and particulate fibre depending upon the shape, orientation and chemical nature. Orientation fibres are used in different angles. From the few decades, carbon and graphite are the common fibre materials used by many weight complex industries. Matrix acts as a bonding element that shields fibre from external break or damage. The main function of the matrix is to distribute and transfer the load to the fibres or reinforcements. There are three types of matrix. Metal matrix composites (MMCs), ceramic matrix composites (CMCs) and polymer matrix composites (PMCs) are the commonly used material for matrix phase. The transformation of load is determined by the bonding interface between the fibre and matrix. The relationship depends on the types of reinforcement material and matrix material and the production technique.



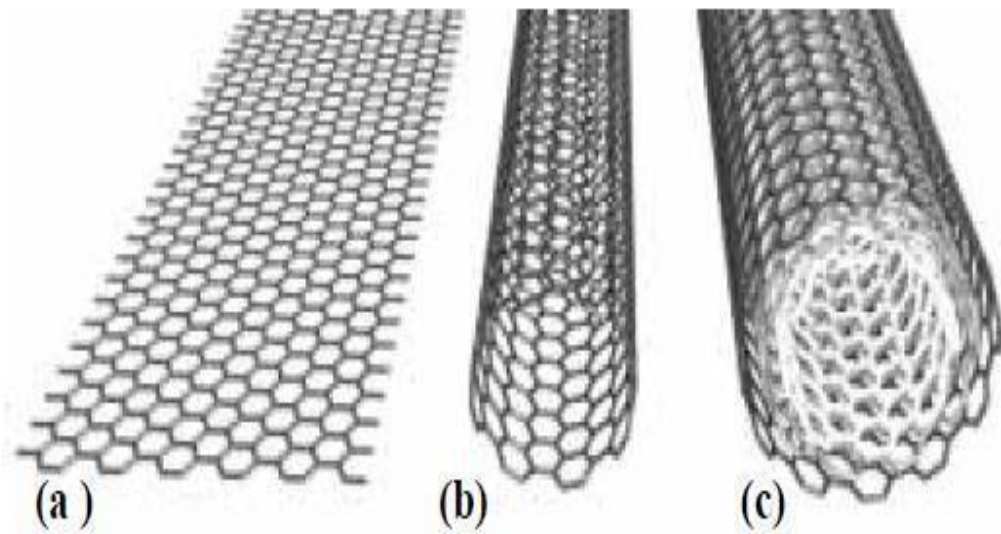
(a) Volume fraction of fibres (Reinforcement)

Fig.1: Volume fraction of fibre

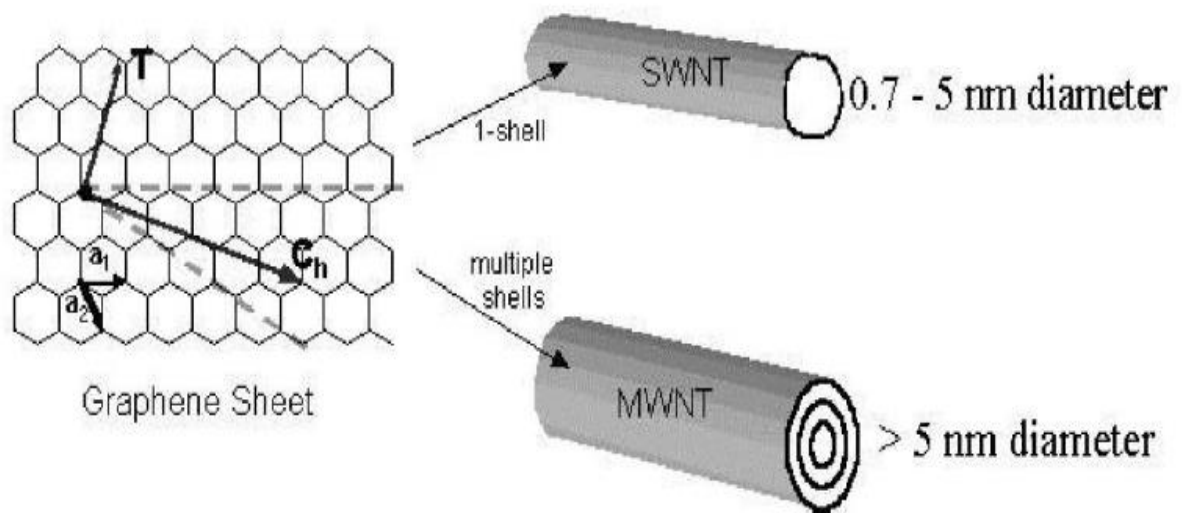
Carbon nanotubes (CNTs) are very high stiffness, resilience and strength, also higher thermal and electrical properties Carbon nanotubes play an important role in the field of engineering. It is cylindrical macromolecules which involve the carbon atoms that are arranged in a periodic hexagonal structure and were invented by Sumio Iijima in 1991. CNT is always used in new field of research for the perfect study of Nano size construction. CNT is used broadly as reinforcing materials at the nanoscale for the development of new nanocomposites, because of its excellent mechanical, thermal and electrical properties. Carbon nanotubes in polymer matrices which can potentially improve the stiffness as well as the strength of the composites very well when compared to those reinforced with conventional carbon fibres. But, retaining these remaining properties at the macro scale positions is a considerable challenge. It is well known that the CNTs have excessive Yield strength, young's modulus, conductivity and elasticity properties. In addition to all these, they have strengths which are 20 times that of the high strength steel alloys, partial denser than aluminium and current carrying capacity is 10000 times that of the copper.

1.2 Types of CNTs

CNTs can be characterized by their structures (a) single walled carbon nanotube (SWNT) (b) multi walled carbon nanotube (MWNT) and (c) double walled carbon nanotube (DWNT). Single walled carbon nanotube is nanometre-diameter tube made up of a single rolled up graphene sheet to form a cylinder and MWNT consisting of multiple rolled up graphene area to form a cylinder but diameter of MWCT is greater than diameter of SWNT is represented in Fig. 2:



(a) A cut- out part of a graphene sheet (b) A single walled CNT (C) A multi walled CNT

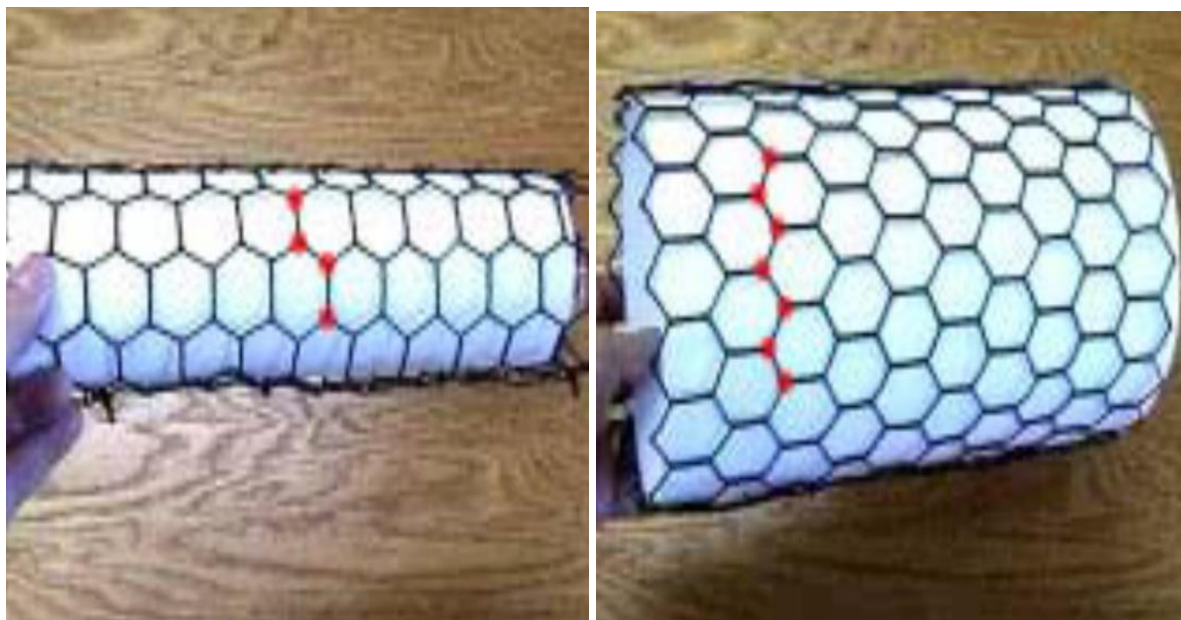


(d) Graphene sheets rolled into SWCNT

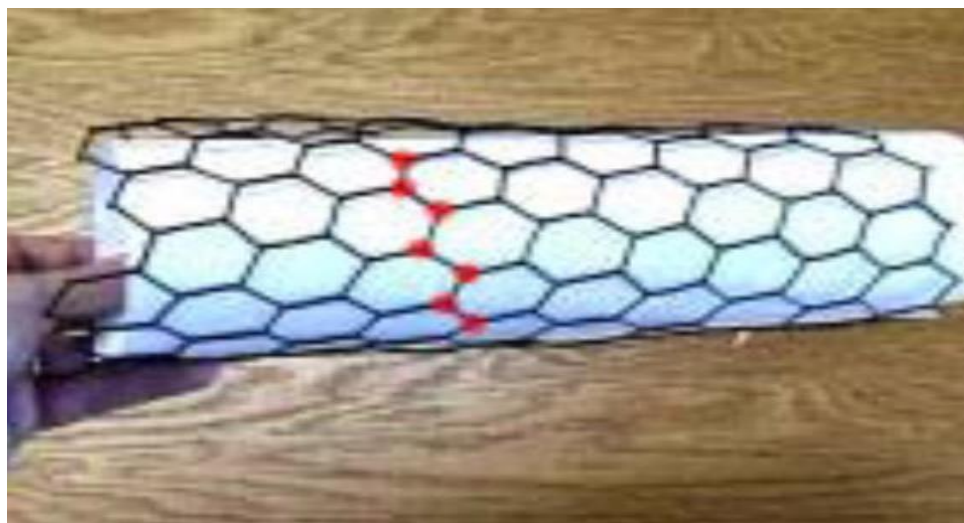
Fig.2: Types of CNTS [36]

1.3 CNTs geometry

CNTs have three exceptional geometrical preparations of carbon atoms. These CNTs can be categorized by how graphene sheet is wrapped into a tube form. Because of physical and mechanical properties of CNTs are depending on its atomic arrangement. There are three types of carbon atom (a) armchair, (b) chiral, and (c) zig-zag as shown in Fig. 3



(a) Arrangement of carbon atom for armchair (b) Arrangement of carbon atom for zig-zag



(a) Arrangement of carbon atoms for chiral

Fig.3:Arrangement of CNTS for armchair,zig-zag and chiral [37]

1.4 Applications of CNTs

CNTs are applied to chemical, mechanical, thermal, electronic and optical field. Carbon nanotube is likely to revolutionize in changed fields such a nanotechnology and material science. CNTs have wide selection of unfamiliar potential applications in many technological fields such as automobile, aerospace, medicine, energy, and chemical industry, in which CNTs may be used as models, gas absorbents, composite fibres material, actuators, substance supports, chemical sensors, probes, nano reactors, nano pipes etc. The key of using CNTs based on FGM is that one can obtain these properties as per the requirement just by varying the distribution and composition of CNTs. That's how one can get directional properties and can control other parameters. Another advantage stated above is the stress concentration free material because the cross-section shows there are no layers inside the material and instead there is a continuous gradation of materials from top to bottom. So, there is no stress concentration and delamination of layers.

1.5 Motivation of the Present Work

The carbon nanotubes CNTs based on composite plate provides highly motivation to the science and technology because of its excellent mechanical, physical, electrical and thermal properties. CNTs are providing effective size, shape, structure, strength to mass ratio, stiffness to mass ratio, wear resistance good elevated temperature properties and the composites based upon CNTs having capability to manufacture guiding mechanical properties and providing capability to mechanism the deformation, forceful reaction of the classification, wear and corrosion of shares etc. In the modern few years, use of composite structures has improved a lot, especially in

aerospace/ aeronautical engineering. The researchers now give their effort on CNTs due to above reason. These structural components are subjected to many types of shared loading and visible to elevated thermal environment during their feature, which may lead to change in the shape of the geometry of arrangement. The changes in panel geometry and the interface with loading condition affect the bending responses significantly. The important aim of this present work is to increase fastening load and control the variability of a structure.

1.6 Aim and Scope of the Present Thesis

The main aim of the thesis are to develop a mathematical model for uniformly distributed single walled carbon nanotubes based on composite plate under various loads and environment temperature using the parametric language in ANSYS 15.0 environment and then calculate its bending responses and free vibration subjected to compressive and tensile load alternately on its adjacent boundaries, based on finite element method. A suitable finite element classical is projected and applied for the discretisation of the composite plate model. It also aims to obtain the effect of uniformly distributed CNT composite plate and other geometrical parameters such as CNT volume fraction, thickness ratio; environment temperature, boundary conditions, compression and tension on the bending responses of the CNTs based composite plate.

CHAPTER 2

LITERATURE REVIEW

Numerous investigated studies and simulations have been performed to study the material properties of the CNT reinforced composites plate. A carbon nanotube is estimated of having young's modulus in the array of tera Pascal (TPA) coupled with high stiffness. Because of these exceptional properties SWCNTs are being widely used in aerospace and biomedical field. The elastic material properties of single walled CNTs and multi-layered carbon nanotubes have been calculated by empirical models.

Zhu et al. [1] computed the free vibration and bending behaviour of the functionally graded carbon nanotube reinforced composite plates (FG-CNTRC) according to the first order shear deformation theory (FSDT) of plate and determines effective physical properties of the nanocomposite plates using extended rule of mixture. Complete parametric studies of the volume fractions of carbon nanotubes and the ratios of width-to-thickness on the bending responses, and fundamental frequencies of the plates and surroundings temperature. Han and Elliott [2] presented the standard molecular dynamics (MD) simulations method to examine the material properties of polymer/fiber composites. Polymer matrices: poly (methyl methacrylate) (PMMA) and poly{(m-phenylenevinylene)- co-[(2,5-dioctoxy-p-phenylene) vinylene]} (PmPV) are used as matrix. Jin and Yuan [3] studied effective elastic modulus of single-walled carbon nanotubes using molecular dynamics (MD) simulations. There are two methods available to evaluate the material properties of CNTs force and energy method. Kumar and Srinivas [4] evaluated the effective material properties of CNTs reinforced polymer by representative volume element method using ANSYS. Rossi and Meo [5] studied the mechanical properties of SWCNT are

recently considered both theoretically and experimentally process. Evaluate mechanical properties as elastic modulus, strain and ultimate strength by finite element method. Alibeigloo and Liew [6] employed three-dimensional theory of resistance, bending behaviour of (FG-CNTRC) rectangular plate exposed to thermo-mechanical loads. Ansari [7] examined the buckling performance of the silicon carbide nanotubes material. Molecular mechanism are generally related to the density functional theory. Murmu and Pradhan [8] observed the buckling behaviours of SWCNTs surrounded in flexible medium using Timoshenko beam theory and Eringen's nonlocal elasticity. Shen [9] computed the nonlinear bending analysis of functionally graded composites plates reinforced by SWCNTs by using the higher order shear deformation plate theory (HSDT) through a Von-Karman based nonlinearity. Popov et al. [10] estimated the elastic properties of triangular close-filled crystal matrices of SWCNTs using analytical words based on a force-constant lattice dynamical model. Ayatollahi et al. [11] estimated the nonlinear mechanical properties of the zigzag and armchair SWNTs bending, under axial and torsional loading conditions using FEM and molecular mechanics. Odegard et al. [12] evaluated a constitutive classical for polymer composite structures reinforced with SWCNTs. Chen and Liu [13] estimated the real mechanical properties of CNTs based on composites using a square representative volume element (RVE) based on the continuum mechanism and with the finite element model (FEM). Shen and Xiang [14] investigated the post buckling of SWCNTs reinforced nanocomposite cylindrical shells under thermo-mechanical loading. The model has been developed based on HSDT panel theories with a von Karman type it is not linearity kinematics. Thai [15] employed a nonlocal tangential deformation beam theory to study the vibration buckling, and the bending. Guo et al. [16] employed an atomic measure finite element model (FEM) to analyse buckling and bending performance of carbon nanotubes (SWCNTs).

Zhang et al. [17] calculated the thermal buckling reactions of carbon nanotubes CNTs using finite element model (FEM). Mohammadimehr et al. [18] investigated the buckling performance of double-walled carbon nanotubes surrounded in an elastic standard under axial compression expending non-local elasticity theory. Sears et al. [19] studied buckling of MWNTs and SWNTs, correspondingly under the axial compressive forces have been studied by MDs, and outcomes compared with those from the investigation of equivalent range assembly using finite element method and Euler buckling theory based upon molecular measure (e.g molecular dynamic forces, montecarlo) and small measure. Vodenitcharova et al. [20] investigated bending and buckling analysis of nanocomposite beam reinforced by SWCNTs, analysed the matrix deformation using Airy stress function. Also, it has been found that adding a quantity of CNTs reinforced in matrix increased load carrying capacity of the structure. Sun and Liew [21] studied a bending buckling behaviour test of SWCNTs using advanced order gradient scale and mesh free technique. Yan et al. [22] investigated the buckling test higher-order Cauchy–Born rule and numerical simulation. Giannopoulos et al. [23] studied the elastic modulus and tangential modulus of the atomistic microstructure of the nanotubes by bond extending, bond angle bending and torsional spin resistance load constants. Lei et al. [24] presented free vibration analysis of FG material nanocomposite panels reinforced by (SWCNTs), using the component-free kp-Ritz method. Aydogdu [25] presented nonlocal beam model free vibration, buckling and bending of nanobeams using the structural and forceful analyses of single-walled carbon nanotubes (SWCNTs). Simsek [26] presented dynamic vibration of a simply reinforced single-walled carbon nanotube (SWCNTs) exposed to a moving simple harmonic load using nonlocal Euler–Bernoulli beam model The effects of nonlocal parameter, the excitation frequency, velocity and aspect ratio. Fiedler et al. [27] presented the potential energy of the CNTs (fibre) in polymers,

the relation among particle volume, separation and size content is described systematically. The subsequent (fracture) mechanical properties of the CNT/epoxy composites material (DWCNT-NH₂) is analysed by transmission electron microscopy (TEM). Lu and Hu [28] adopted Computational model for calculating mechanical properties of single-walled carbon nanotubes (SWCNTs) as it is an influential tool relative to the tentative difficulty. and investigated the things of diameters of helicity on young's modulus and the tangential modulus of SWCNTs. Yu et al. [29] studied the carbon nanotubes (CNTs) and the fibre and polymer matrix boundary coating the chemical vapour deposition (CVD) method using methyltrichlorosilane (MTS). Properties of the CNTs on mechanical and thermal effects of the composite material calculate by three-point flexible test, single-edge notched beam (SENB) test. Formica et al. [30] employed the vibrational effects of carbon nanotubes the Eshelby–Mori–Tanaka the single-walled carbon nanotubes (SWCNTs).The composite panel are made of a purely isotropic elastic material introducing matrix of three dissimilar types (concrete, rubber, and epoxy). Odegard et al. [31] developed the assembly-property relations of Nano-structured resources. This technique attends as a link between computational solid mechanics and chemistry by replacing separate molecular arrangements with equivalent-field models. Calculate the effective-field geometry and bending inelasticity of a graphene sheet subjected to cylindrical bending. Volcov et al. [32] studied the bending buckling analysis of single-walled carbon nanotubes (SWCNTs) based on thermal conductivity of CNTs. microscopic simulations and atomistic. Nonequilibrium it is used in molecular dynamics (MD) simulations of the thermal conductance through a separate buckling kink in a (10, 10) armchair shape CNT. Ma et al. [33] investigated the surface, diffusion and interfacial properties of carbon nanotubes (CNTs), the functionalization efficiently constrain the re-agglomeration of CNTs through the remedial of resin. These finalising properties along with

enhanced interfacial linkage between the matrix and reinforced CNTs. Liu and Chen. [34] Presented the progresses in the boundary element technique for carbon nanotube (CNTs) based on composites and finite element method to demonstrate the efficiency of BEM. Coleman et al. [35] presented a review paper to evaluate the mechanical properties of carbon nanotube–polymer composites.

Based on the above literature, it is clear that many attempts have been made to study the mechanical free vibration and bending behaviour of FG-CNTRC but the studies with temperature dependent material properties were very rare. Hence, the present research work focus on the analysis of the mechanical free vibration and bending analysis of uniformly distributed (UD) and FG-CNTRC with temperature dependent material properties. A simulation model is developed using ANSYS parametric design language (APDL) in ANSYS environment.

CHAPTER 3

GENERAL MATHEMATICAL FORMULATION

3.1 Molecular Dynamics Simulation

The modelling of mechanical properties of Nano composites is done by the help of molecular dynamics simulation (MDs) by using direct methods, and the other method used is finite element simulation technique by “continuum” methods. Molecular dynamics is the utmost in depth molecular simulation method that computes the motion of distinct molecules. Coupled Newton’s equation of motion, it defines the place and momentum, are explained for a huge number of atoms in separated bunch or in the bulk by the use of periodic boundary conditions. Molecular dynamics usually contains of three components.

- (1) A traditional of the first conditions (e.g., the initial positions and also the velocities of all atoms in the system)
- (2) The interface potential energy to characterise the all the forces among all the atoms.
- (3) The development of scheme in the time by statistically explaining a set of classical Newtonian equations of the motion for totally atoms in the system. In the year 1997, Cornwell et al. used the molecular dynamics to calculate the elastic properties of single-walled carbon nanotubes SWCNTs. In current areas, molecular dynamics simulation have been broadly used in expecting materials properties of CNTs and nanotubes reinforced composites material , graphite/epoxy nanocomposites, and the other nanocomposites. Molecular dynamics simulation contains a suitable selection of the interaction potential energy of particles, geometric combination, periodic edge conditions, and this is the controls of temperature and pressure for

simulator materially meaningful thermodynamic groups. The relations potentials energy together with their constraints forms a force field that explains in detail how the particles in a system interact with each other particles. Such a dynamic ground can be attained by the quantum system and empirical method or quantum-empirical method. The standards used for choosing a dynamic field contain the precision, computational speed and transferability. The total potential energy U may contain of a number of non-bonded and bonded collaboration terms.

$$\sum U = \sum U_{bond} + \sum U_{angle} + \sum U_{torsion} + \sum U_{iversion} + \sum U_{non-bonded} \quad (3.1)$$

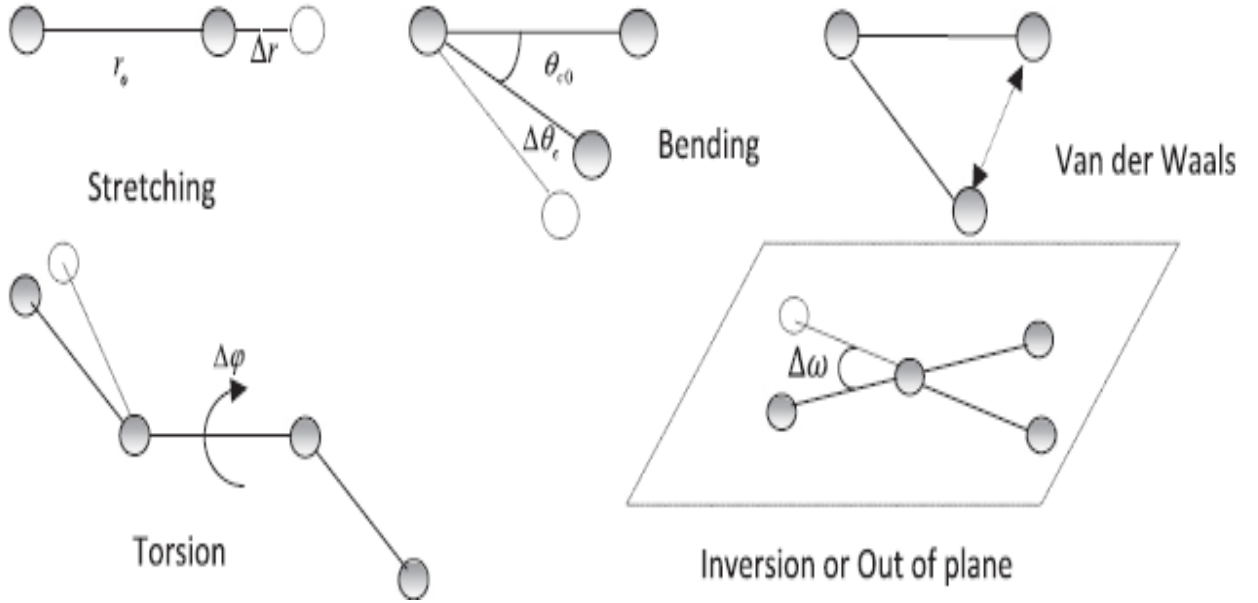


Fig.4: the interatomic interaction in molecular dynamics notion.[5]

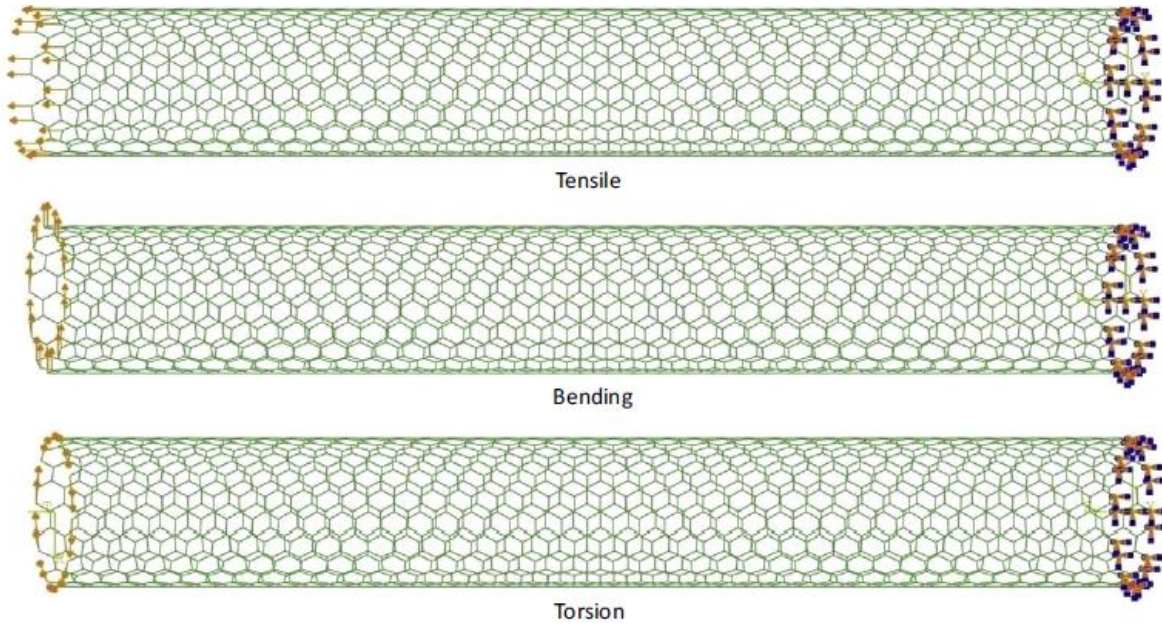


Fig.5: boundary loading conditions for SWCNT armchair (10,10) [11]

3.1.1 Structure of carbon nanotube

Single-walled nanotubes SWCNTs are designed by folding a graphene sheet to procedure a hollow tube that is collected of the hexagonal shape carbon circle units, they are usually referred as graphene units. The important carbon nanotube structure which can be categorised into three types: (1) Armchair of atoms (2) zigzag of atoms and (3) chiral of atoms in relations of their helicity. Fig. [6] Shows a part of a single graphite plane it can be converted into a carbon nanotube by rolling a tube. To designate this construction, a chiral direction is given by the equation $OA = na_1 + ma_2$, where a_1 and a_2 are unit directions for the graphene sheet, there are two integers of n and m , along with a chiral angle θ that is the angle of the chiral direction with respect to the x co-ordinate shown in Fig.[6] The chiral direction, OA will be represented by (n, m) which will also identify the structure of the CNT. The direction OB is perpendicular to the direction OA . To geometry a CNT, we cut off the squares $OABO$ and roll it

into a tube with OB and ABO coinciding each other. The relationship between the co-ordinate of integers (n, m) and then nanotube radius, R, and θ chiral angle is given by

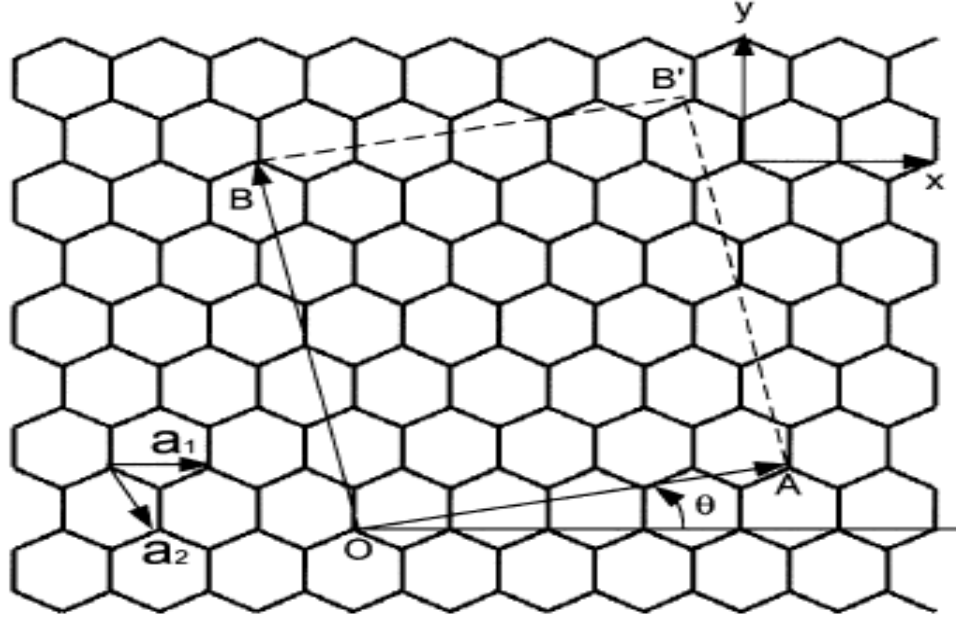


Fig.6: The graphite plane of nanotube surface coordinates.[38]

$$R = \frac{\sqrt{3}a_{c-c}(\sqrt{m^2 + n^2 + m.n})}{2\pi} \quad (3.2)$$

$$\theta = \tan^{-1} \left[\frac{\sqrt{3}n}{(2m + n)} \right] \quad (3.3)$$

The properties of the geometry of carbon atom. According to θ

Armchair: $m=n$, $\theta = 30^\circ$

Zigzag: m or $n=0$, $\theta = 0^\circ$

Chiral: $0^\circ < \theta < 30^\circ$

3.2.2. Force fields and total potential energy

The molecular dynamics MD simulation methods are deterministic which is based on the Newton's second law of motion, $F = ma$ here F is the force applied on an atom, m is the mass of atoms and a is its acceleration of atoms. From information of the force on each atom, the acceleration of the each atom in the structure can be evaluated. The mathematical addition of the equations of motion produces a path that terms the positions, velocities and accelerations of each atom with respect to time. From this path, the mean values of properties can be calculated. The atomic relationship is explained by force potentials connected with Bonding and nonbonding phenomena. The relation potential energy is the sum of bonding energy and non-bonding energy.

$$\sum U = \sum U_{bonded} + \sum U_{non-bonded} \quad (3.4)$$

For carbon nanotubes, this nonbonding duration is mostly the energy of van-der-Waals force, the normally have a weak inspiration on the totally mechanical behaviour between the atomic connections of the carbon microstructure. The van-der-Waals force is most regularly modelled using the Lennard-Jones 6-12 potential function.

$$\sum P_{vander-waals} = \sum_{nonbondedpair} \left(\frac{A_{ij}}{r_{ij}^{12}} - \frac{C_{ij}}{r_{ij}^6} \right) \quad (3.5)$$

Where A and C are the atom-type reliant on constants. $r_{ij} = |r_i - r_j|$ is the distance between two molecules, i and j, and r_i and r_j are the position directions of i_{th} and j_{th} atom. The main part of the overall potential energy, the bonding energy, is a sum of three changed connections among atoms: bond stretching, bond bending, and bond torsion. Two potential energy are negligible.

$$U_{bonded} = U_{bond-stretch} + U_{angle-bend} + U_{torsion} \quad (3.6)$$

Where U is generally used potential energy functions are given by the equation

$$U_{bond-stretch} = \sum_{1,2\ pairs} K_s (r_{ij} - r_0)^2 \quad (3.7)$$

$$U_{angle-bend} = \sum_{angles} K_\theta (\theta - \theta_0)^2 \quad (3.8)$$

$$U_{torsion} = \sum_{1,4\ pairs} K_\phi (1 - \cos(n\phi + \phi_0)) \quad (3.9)$$

Where r_0 is equilibrium distance of bond. There are three type of this bond, K_s is the spring force of bond, K_θ is the force of bending, and K_ϕ is the torsion force, this is the ideal part for this bond type, and where n is periodicity of the bond. The constants are firm as approximations for the complete quantum relations of the electron wave roles fundamental the interaction of unlike carbon atoms. A statistical program is generated to evaluate the mutual relations forces determined by the slope of the overall potential energy of a single-walled nanotube, $F = -\nabla U$ Applying Newton's Second Law of motion, the Verlet technique is used for carrying out the addition at definite time steps to get atom path.

There are two methods to evaluate the elastic properties of carbon nanotubes.

(1) Force method (2) Energy method

(1) Force method:

The elastic properties of CNTs are recorded by direct computation of the mean dynamic developed between the carbon atoms in the nanotube. Virial theorem, a force method is used for calculation of the effective elastic modulus in longitudinal direction. This equation is given by

$$\sigma_{\alpha\beta} = -\frac{1}{2V_0} F_{ij}^{\beta} r_{ij}^{\alpha} \quad (3.10)$$

Where $\sigma_{\alpha\beta}$ is the average atomic level stress tensor in the Cartesian Coordinates, F_{ij}^{β} is interatomic forces with bonding and nonbonding forces between two molecules i and j, r_{ij}^{α} is the distance between two atoms and V_0 is the initial volume of the carbon nanotube, this is a hollow cylinder. $V_0 = 2\pi h L r$ where h is the assumed thickness of hollow cylinder, L is length of tube wall and r is radius of tube wall.

(1) Energy method:

The second derivative of the potential energy with respect to the strain under each bend approach is utilized for calculation of elastic modulus.

$$C_{ijkl} = \frac{1}{V_0} \frac{\partial^2 U}{\partial \varepsilon_{ij} \partial \varepsilon_{kl}} \quad (3.11)$$

Where C_{ijkl} is the fourth-order tensor of elastic constants and ε_{ij} is the strain tensor. and U is potential energy.

The potential energy is used in energy method under small strain deformation equation is given

by

$$U = U_0 + \frac{1}{2} V_0 C_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \quad (3.12)$$

Where U is the overall potential energy at the equilibrium and U_0 is initial potential energy at the equilibrium before bend is applied.

The common elastic features of carbon nanotubes will now be discussed. Due to the hexagonal symmetry properties in the tube surface of nanotube, the nanotube transverse isotropy in the θ - z plane, this is independent of five elastic constants in the stress and strain relationships.

$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \end{Bmatrix} = \begin{bmatrix} C_{11} & C_{13} & C_{13} \\ C_{13} & C_{33} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{bmatrix} \begin{Bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \end{Bmatrix} \quad (3.13)$$

$$\tau_{\theta z} = G_{\theta z} \gamma_{\theta z}, \tau_{rz} = G_{rz} \gamma_{rz}, \tau_{r\theta} = G_{r\theta} \gamma_{r\theta} \quad (3.14)$$

Where $G_{\theta z} = \frac{E_z}{2(1+\nu_{\theta z})}$

The equation is expressed in terms of engineering constants as

$$\begin{Bmatrix} \sigma_{rr} \\ \sigma_{\theta\theta} \\ \sigma_{zz} \end{Bmatrix} = \begin{bmatrix} \frac{1}{E_r} & -\frac{\nu_{zr}}{E_z} & -\frac{\nu_{zr}}{E_z} \\ \frac{\nu_{zr}}{E_z} & \frac{1}{E_z} & -\frac{\nu_{\theta z}}{E_z} \\ \frac{\nu_{zr}}{E_z} & \frac{\nu_{\theta z}}{E_z} & \frac{1}{E_z} \end{bmatrix} \begin{Bmatrix} \varepsilon_{rr} \\ \varepsilon_{\theta\theta} \\ \varepsilon_{zz} \end{Bmatrix} \quad (3.15)$$

(1) Evaluation of elastic modulus E_I and Poisson $\nu_{z\theta}$

The axial young's modulus E_z and the Poisson ratios, ν_z the atoms are displaced by

$$u_{zz} = \varepsilon_{zz}^0 z \text{ the average strain and stresses are: } \varepsilon_{zz} = \varepsilon_{zz}^0$$

$$\sigma_{zz} \neq 0, \text{ any other } \sigma_{ij} = 0$$

The MD simulation, the longitudinal elastic modulus, E_z , can be evaluated by force and energy method.

$$(a) \text{ Force method} \quad E_z = \frac{\sigma_{zz}}{\epsilon_{zz}^0} \quad (3.16)$$

$$(b) \text{ Energy method} \quad E_z = \frac{1}{V_0} \frac{\partial^2 U}{\partial \epsilon_{zz}^0{}^2} \quad (3.17)$$

$$(c) \text{ Poisson's ratio is obtained as: } \nu_{z\theta} = -\frac{\epsilon_{\theta\theta}}{\epsilon_{zz}^0} \quad (3.18)$$

(2) Calculation of E_2 and $\nu_{\theta z}$

The radial displacement $u_r = \epsilon_{\theta\theta}^0 r$ is applied to every atom of carbon nanotube then we are obtain only a hoop stress $\epsilon_{\theta\theta} = \epsilon_{\theta\theta}^0$

$\sigma_{\theta\theta} \neq 0$, any other $\sigma_{ij} = 0$

The MD simulation, the transverse elastic modulus, E_θ

$$(a) \text{ Force method} \quad E_\theta = \frac{\sigma_{\theta\theta}}{\epsilon_{\theta\theta}^0} \quad (3.19)$$

$$(b) \text{ Energy method} \quad E_\theta = \frac{1}{V_0} \frac{\partial^2 U}{\partial \epsilon_{\theta\theta}^0{}^2} \quad (3.20)$$

$$(c) \text{ Poisson's ratio is obtained as: } \nu_{\theta z} = -\frac{\epsilon_{zz}}{\epsilon_{\theta\theta}^0} \quad (3.21)$$

(3) Calculation of the rotational shear modulus $G_{\theta z}$ and the displacement mode $u_\theta = \gamma_{\theta z}^0$

$\gamma_{\theta z} = \gamma_{\theta z}^0$, any other $\epsilon_{ij} = 0$

$\tau_{\theta z} \neq 0$, any other $\sigma_{ij} = 0$

$$(a) \text{ Force method} \quad G_{\theta Z} = \frac{\tau_{\theta Z}^0}{\gamma_{\theta Z}^0} \quad (3.22)$$

$$(b) \text{ Energy method} \quad G_{\theta Z} = \frac{1}{V_0} \frac{\partial^2 U}{\partial \gamma_{\theta Z}^0{}^2} \quad (3.23)$$

(4) Calculation C_{23} and C_{33}

The carbon atoms are under deformation $u_z = \varepsilon_{zz}^0 z$ and lateral displacement are constrained

$$\varepsilon_{zz} = \varepsilon_{zz}^0, \text{ any other } \varepsilon_{ij} = 0$$

This is relationships stress and strain; C_{23} and C_{33} are given by

$$(a) \text{ Force method} \quad C_{23} = \frac{\sigma_{\theta\theta}}{\varepsilon_{zz}^0} \quad (3.24a)$$

$$C_{33} = \frac{\sigma_{zz}}{\varepsilon_{zz}^0} \quad (3.24b)$$

$$(b) \text{ Energy method} \quad C_{33} = \frac{1}{V_0} \frac{\partial^2 U}{\partial \varepsilon_{zz}^0{}^2} \quad (3.25)$$

Where C_{13} can be evaluation using a force method, this elastic modulus is small value, the determination of C_{13} is not attempted.

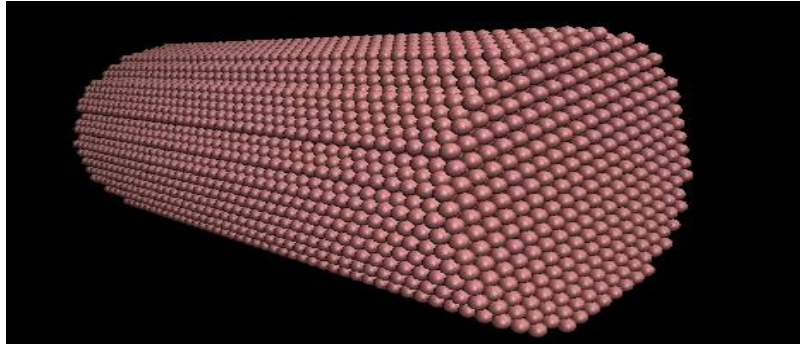


Fig (a) Solid CNT through MD

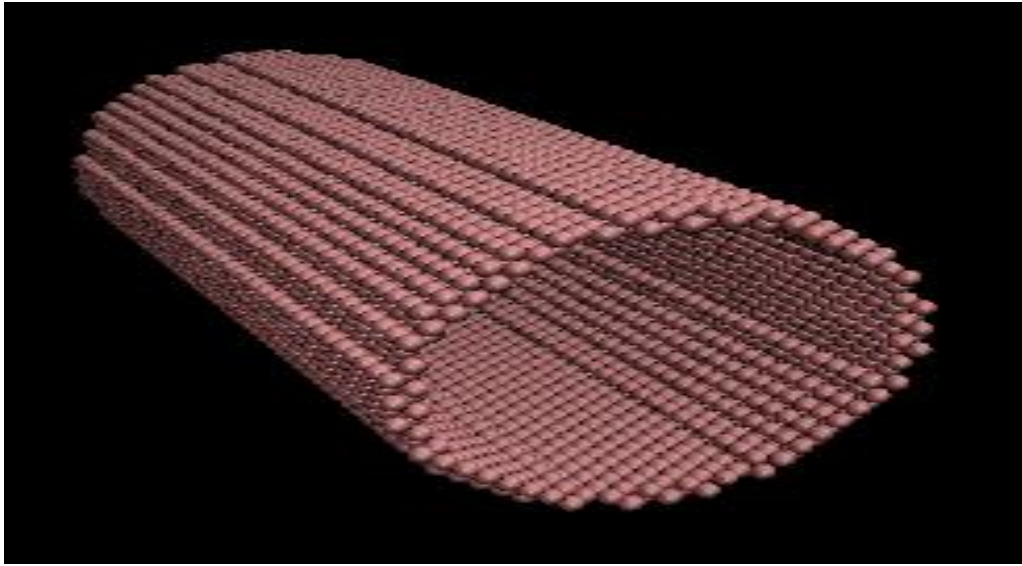


Fig (b) Hollow CNT through MD

Fig.7: Solid and Hollow CNTs through MD

3.2 Finite Element Method and ANSYS

Nowadays the advancement in the technology, the design engineering method is also close to precision, as the finite element model (FEM) is used broadly and capable to drawing the complicated structure and this method is very important tool for the designing process of any shape and construction. It shows an important role in forecasting the responses of different products, parts, assemblies and subassemblies. The FEM is very extensively used by all advanced field in which save their huge time of prototyping with decreasing the cost due to physical check and increases the revolution at a faster and more accurate path. There are various optimized finite element analysis (FEM) tools are obtainable in this market and ANSYS parametric is one of them (FEM) is acceptable to several industries and analysts.

Nowadays, ANSYS is creature used in different engineering areas such as power generation, electronic devices, transportation, and household appliances as well as to analyse the

vehicle simulation and in aerospace industries. ANSYS gradually enters into the number of fields which is making it convenient for the fatigue analysis, nuclear power plant and medical applications. ANSYS is also very useful in structural analysis.

SHELL281 element description.

The shell element is using for bending analysis. The element has eight-node with six degrees of freedom for each node. Shown in fig.8 is select from the element library of ANSYS 15. That is translations in the nodal x, y and z directions.

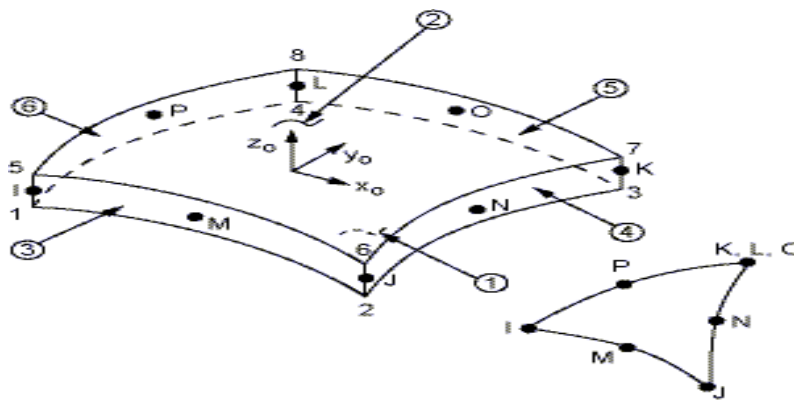


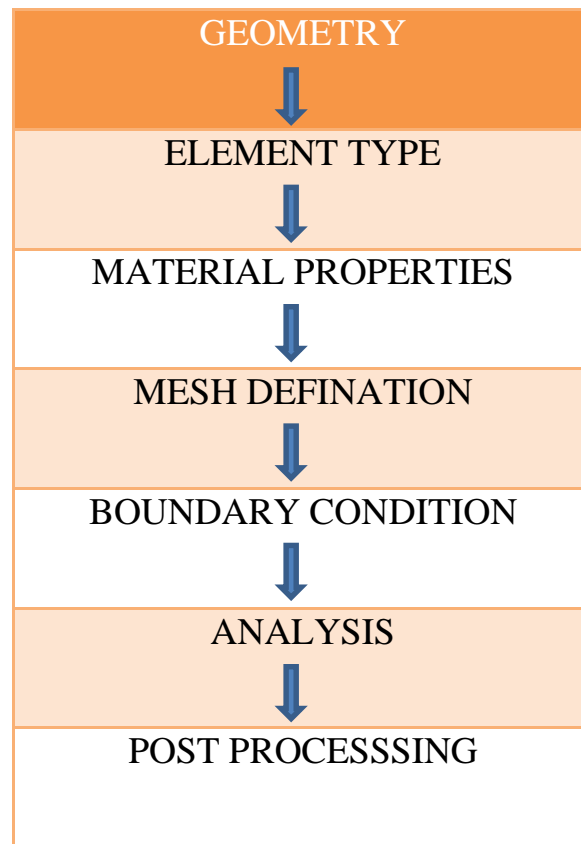
Fig. 8: Shell 281 element description.

x_0 = The x-axis of element co-ordination is not provided.

x = The x-axis if element co-ordination is provided.

A layout of procedure in ANSYS:

:



3.3 Carbon Nanotube Composites Plate

In this paper, UD- CNT composite plate using length a , width b and depth are measured. UD-CNT composite plate represents the uniform supply the functionally graded spreading of carbon nanotubes in the depth direction of the composite plates. The effective material properties of the two-part Nano composites, it is the rule of mixture of CNTs and an isotropic polymer and can be calculated according to the extended rule of mixture. Due to the relaxed and suitability, in the work the rule of mixture was active by presenting CNT efficiency constraints and effective material properties of the CNTRC plates is given by the equation.

$$E_{11} = \eta E^{CNT} V_{CNT} + E^m V_m \quad (3.26)$$

$$\frac{\eta_2}{E_{22}} = \frac{V_{CNT}}{E_{22}^{CNT}} + \frac{V_m}{E^m} \quad (3.27)$$

$$\frac{\eta_3}{G^{12}} = \frac{V_{CNT}}{G_{12}^{CNT}} + \frac{V_m}{G^m} \quad (3.28)$$

Where, E_{11}^{CNT} , E_{22}^{CNT} and G_{12}^{CNT} are the elastic constants of SWCNT and E^m , G^m are characterize the elastic properties of the matrix. η_1, η_2 and η_3 are the CNT effective parameters and it can be estimated by the effective material properties of CNTRC based on the rule of mixture and molecular dynamic (MD) simulation. V_{CNT} And V_m are the volume fractions of the fibre and volume fraction of matrix. E_{11} And E_{22} are the effective Young's modulus of carbon nanotubes reinforced composite plates in the main material coordinates, G_{12} , G_{13} and G_{23} are the tangential modulus, ν_{12} and ν_{21} are Poisson's ratios and α_{11} and α_{22} are thermal expansion coefficients.

In the same way, the thermal extension coefficients, α_{11} and α_{22} individually, in this type the longitudinal and transverse ways, Poisson's ratio ν_{12} and ρ the density of the Nano composite plates find out in the same way as relation between the CNT and matrix volume fractions is shown as.

$$V_{CNT} + V_m = 1 \quad (3.29a)$$

$$\nu_{12} = V_{CNT}^* \nu_{12}^{CNT} + V_m \nu^m \quad (3.29b)$$

$$\rho = V_{CNT} \rho^{CNT} + V_m \rho^m \quad (3.29c)$$

$$\alpha_{11} = V_{CNT} \alpha_{11}^{CNT} + V_m \alpha^m \quad (3.30a)$$

$$\alpha_{22} = (1 + \nu_{12}^{CNT}) V_{CNT} \alpha_{22}^{CNT} + (1 + \nu^m) V_m \alpha^m - \nu_{12} \alpha_{11} \quad (3.30b)$$

Here, ν^{CNT} and m are Poisson's ratio of CNT and matrix, respectively and α_{11}^{CNT} , α_{22}^{CNT} and α^m are the thermal expansion coefficients of the CNT and matrix.

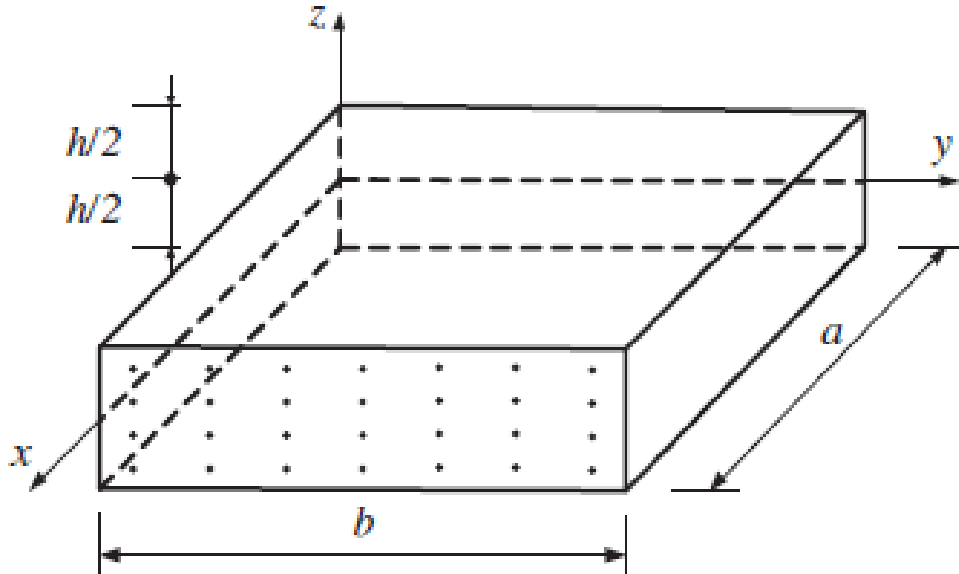


Fig.9: Carbon nanotube reinforced composites plate. [1]

3.4 Free vibration of CNTC plate

The vibration which occurs when the mechanical system is set off with an initial input and then permissible to vibrate freely. As for Examples this physical type of vibration are pulling of a child back on the swing and then letting go. The mechanical system then vibrates at one or more of its "natural frequency" and damp down to zero.

In a free vibration analysis, the CNT composite plate is assumed to undergo a harmonic motion and the recorded eigenvalue and eigenvector equations are given by

$$(K_0 - \omega^2 M)d = 0 \quad (3.31)$$

Where K_0 is the global stiffness matrix, M is the global mass matrix and ω is normal frequency are calculated by assembling the element mass matrix M^e

$$M^e = \int_{\Omega^e} [\psi^e]^T \rho [\psi^e] d\Omega \quad (3.32)$$

$$[\rho] = \begin{bmatrix} J_0 & 0 & 0 & J_1 & 0 \\ 0 & J_0 & 0 & 0 & J_1 \\ 0 & 0 & J_0 & 0 & 0 \\ J_1 & 0 & 0 & J_2 & 0 \\ 0 & J_1 & 0 & 0 & J_2 \end{bmatrix} \quad (3.33)$$

Where J_0, J_1 and J_2 are the normal, coupled normal-rotary and rotary inertial coefficient respectively.

$$(J_0 J_1 J_2) = \int_{-h/2}^{h/2} \rho(Z_1) (1, Z_1, Z_1^2) \quad (3.34)$$

The non-dimensional natural frequency equation is given by

$$\varpi = \omega(a^2/h) \sqrt{\rho^m/E^m} \quad (3.35)$$

3.5 Bending Analysis of CNTC plate

Bending analysis is nothing but the geometrical shape change of structural component and usually curve in nature. Numerous analyses have been reported in the literature on the bending analysis by taking the geometric matrix and the stiffness matrices in von-Karman sense based in various theories such as classical plate theory and the shear deformation theories. Lots of literature are there on carbon nanotube of the composite plate due to bending loadings. A few of them are discussed here.

The generalized displacements at any point within an element Ω^e are approached.

$$U_o^h(X, t) = \sum_{i=1}^m \psi_i^e(X) d_i^e(t) \quad (3.36)$$

Where ψ_i^e is the lagrangian interpolation functions and d^e is expressed as nodal displacements of the element Ω^e . The finite element equations of CNT composites plates subjected to a uniformly distributed transverse load is given by

$$Kd = F \quad (3.37)$$

Where K is the global stiffness matrix and F is load vector these are computed by assembling.

CHAPTER 4

RESULT AND DISCUSSION

4.1 Evaluation of material properties of carbon nanotubes using MD simulation

In MD simulation, this is used parameters of length, diameter and different temperature. We are deciding of no of atoms and no of iteration.

Table.1: The comparison of material properties in molecular dynamics.

Temperature (°K)	Material properties	Zhu et al. [1]	Present (MD)
300	E_I	5.6466	5.543
500	E_I	5.5306	5.486
700	E_I	5.4744	5.368

4.2 Effect of volume fraction on the non-dimensional elastic modulus of CNT

CNT geometry is generally influenced by the chiral vector (n, m), the conclusion of chirality on elastic modulus as estimated by Halpin–Tsai method [35]. It is realized that zigzag CNT with chiral vector (10, 0) gives higher non-dimensional elastic modulus. Various numerical examples are discussed in this section and they are validated with reference. Fig.10 shows the effect of volume fraction on the non-dimensional elastic modulus. In MD simulation, young's modulus ($E_Z=1208\text{GPa}$) and polymer matrix ($E_m=2.5$) are used.

Table.2: Comparison of non-dimensional elastic modulus (E_z/E_m) for different volume fraction.

Volume	Kumar and	Present	Kumar and	Present	Kumar and	Present
	Srinivas [4]	(MD)	Srinivas [4]	(MD)	Srinivas [4]	(MD)
Fraction (%)	CNT (10,0)	CNT(10,0)	CNT(10,5)	CNT(10,5)	CNT(10,10)	CNT(10,10)
1	2.06	2.23	1.993	2.01	1.75	1.75
2	3.31	3.61	2.77	3.07	2.34	2.52
3	4.48	4.95	3.67	4.00	3.01	3.29
4	5.64	6.33	4.66	5.04	3.64	4.09
5	6.73	7.73	5.56	6.02	4.31	4.97

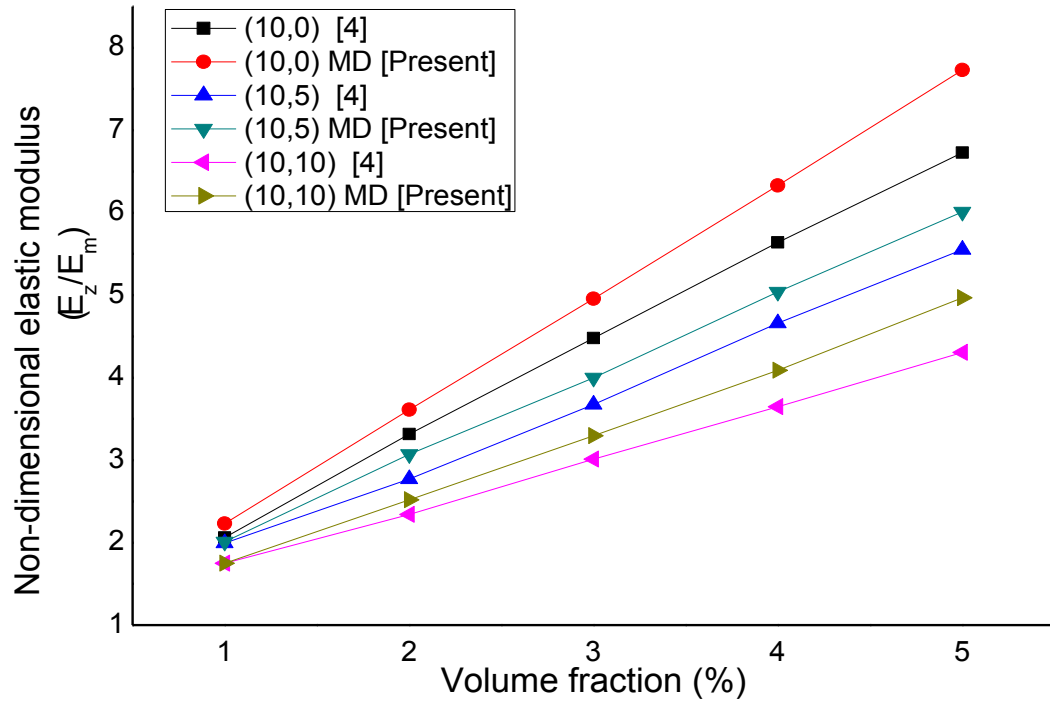


Fig.10: Variation of non-dimensional elastic modulus of CNT composite plate for different types of fibres.

Table.3: The material properties of (10, 10) SWCNT ($L = 9.26$ nm, $R = 0.68$ nm, $h = 0.067$ nm.

$$\nu_{12}^{mt} = 0.175. [1]$$

Temperature (°K)	E_1	E_2	G_{12}	$\alpha_{11} (10^{-6} / ^\circ\text{K})$	$\alpha_{22} (10^{-6} / ^\circ\text{K})$
300	5.6466	7.0800	1.9445	3.4584	5.1682

4.3 Numerical illustrations.

In present analysis the PmPV is used as the matrix and the material properties of PmPV are $\nu^m = .34$, $\rho^m = 1.15 \text{ g/cm}^3$, and $E^m = 2.1 \text{ GPa}$ at room temperature (300K). SWCNTs are used as fibre material for bending and free vibration analysis and the material properties are present in table 3. The extended rule of mixture used to evaluate the material properties of CNTRC plate. Effectiveness parameter of CNT $\eta_1 = 0.149$ and $\eta_2 = 0.934$, for $V_{CNT} = 0.11$, $\eta_1 = 0.150$ and $\eta_2 = 0.941$ for the case of $V_{CNT} = 0.14$, and $\eta_1 = 0.149$ and $\eta_2 = 1.381$ for $V_{CNT} = 0.17$. We assume that $G_{23} = G_{13} = G_{12}$ and $\eta_3 = \eta_2$. The width to thickness ratio ($a/h = 10, 20$ and 50) and volume fraction are taken as design parameter of bending analysis. The thickness is taken to be 2.0mm . The uniformly distributed carbon nanotube composites square plate ($a/b = 1$) is considered with boundary conditions (a) SSSS, (b) CCCC and (c) SCSC. Uniformly distributed load ($q_0 = -0.1\text{MPa}$) used to calculate the bending behaviour of the composite plate.

4.3.1 Bending analysis

For bending analysis, non-dimensional central deflection is obtained using $\bar{W} = W / h$ formula. Figs.11-13 shows the non-dimensional central deflection of CNT composite plate for different support condition under uniformly distributed load. From figures it is clearly shown that the non-dimensional central deflection of composite plate increasing with thickness ratio (a/h) and also shown that non-dimensional central deflection is increasing with volume fraction. For better understand three table are present.

Table.4: The non-dimensional central deflection for different thickness ratio (a/h) validation using volume fraction (SSSS).

a/h	Zhu et al.[1] ($V_{CNT} = 0.11$)	Present	Zhu et al.[1] ($V_{CNT} = 0.14$)	Present	Zhu et al.[1] ($V_{CNT} = 0.17$)	Present
10	0.003739	0.00373	0.003306	0.003315	0.002394	0.003015
20	0.003628	0.03625	0.03001	0.0301	0.02548	0.0259
30	0.0167	0.161	0.1292	0.1295	0.104	0.1045
40	0.488	0.484	0.381	0.385	0.311	0.315
50	1.155	1.153	0.9175	0.9195	0.7515	0.7645

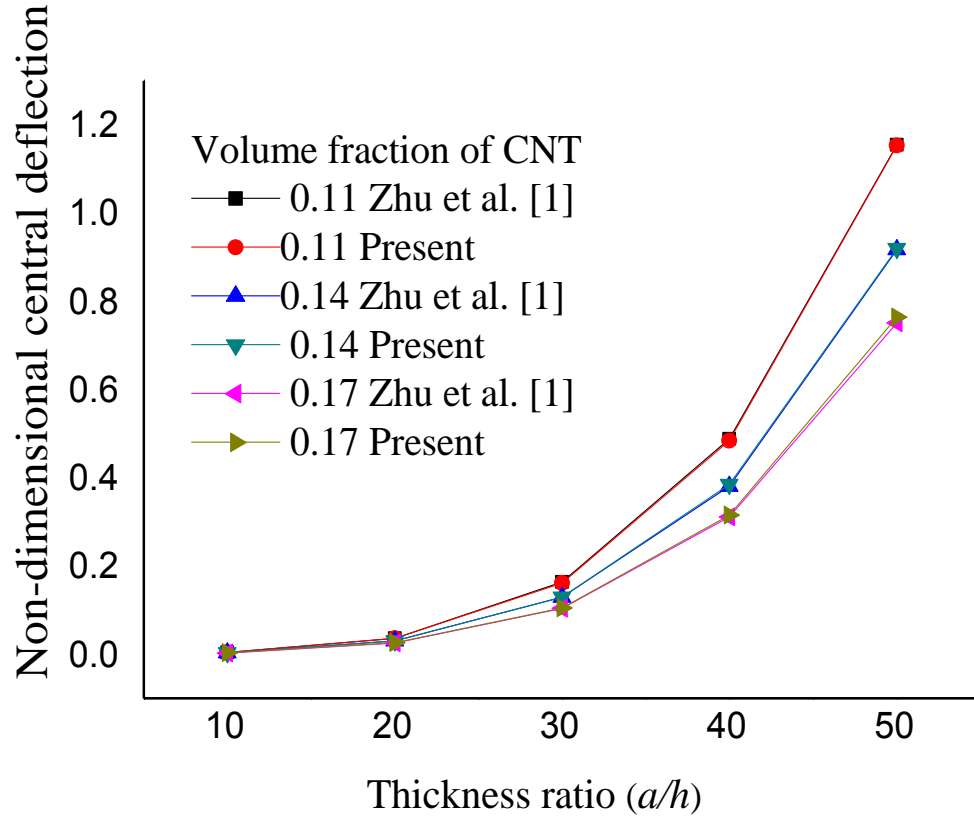


Fig.11: Effect of thickness ratio on non-dimensional central deflection.

Table.5: The non-dimensional central deflection for different thickness ratio (a/h).

(a) CCCC

a/h	($V_{CNT} = 0.11$)	($V_{CNT} = 0.14$)	($V_{CNT} = 0.17$)
10	2.2200E-03	2.0950E-03	1.9850E-03
20	1.3350E-02	1.1900E-02	1.0900E-02
30	4.5250E-02	3.8400E-02	2.9150E-02
40	1.1800E-01	9.2500E-02	7.6500E-02
50	2.6050E-01	2.1350E-01	1.8250E-01

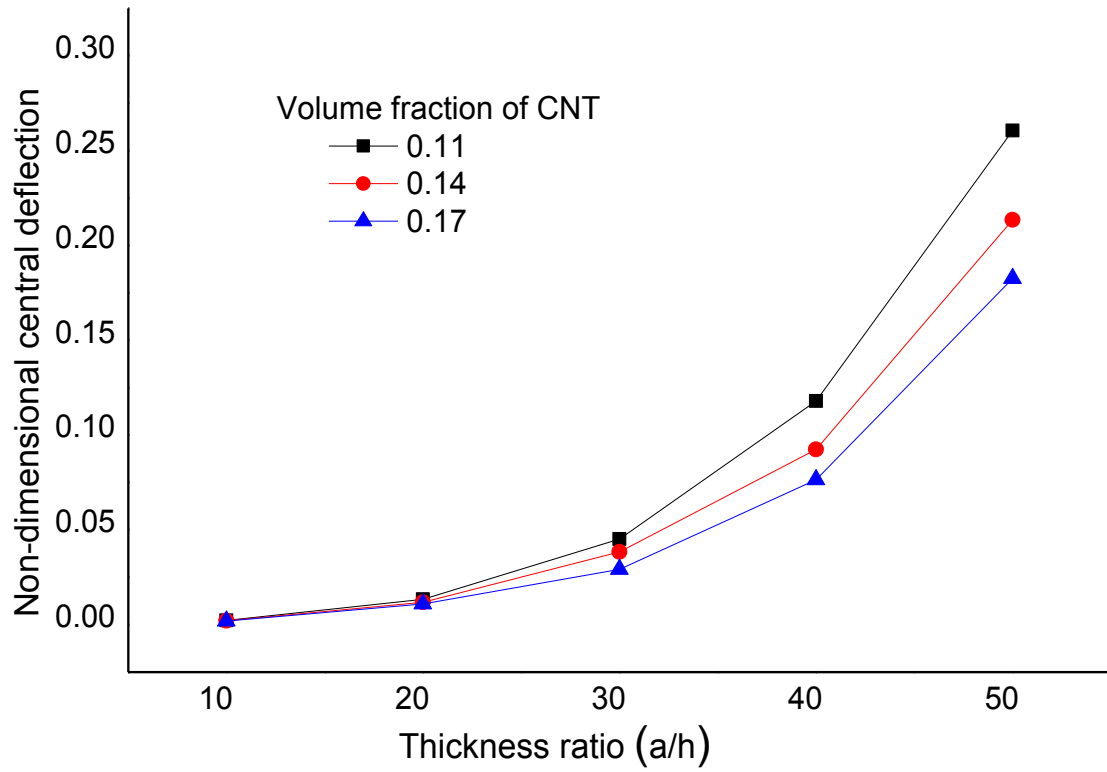


Fig.12: Effect of thickness ratio on non-dimensional central deflection

Table.6: The non-dimensional central deflection for different thickness ratio (a/h).

(b)SCSC

a/h	($V_{CNT}=0.11$)	($V_{CNT}=0.14$)	($V_{CNT}=0.17$)
10	3.32E-03	2.98E-03	2.74E-03
20	3.39E-02	2.86E-02	2.49E-02
30	1.53E-01	1.45E-01	9.85E-02
40	4.60E-01	3.73E-01	2.98E-01
50	1.10E+00	8.91E-01	7.50E-01

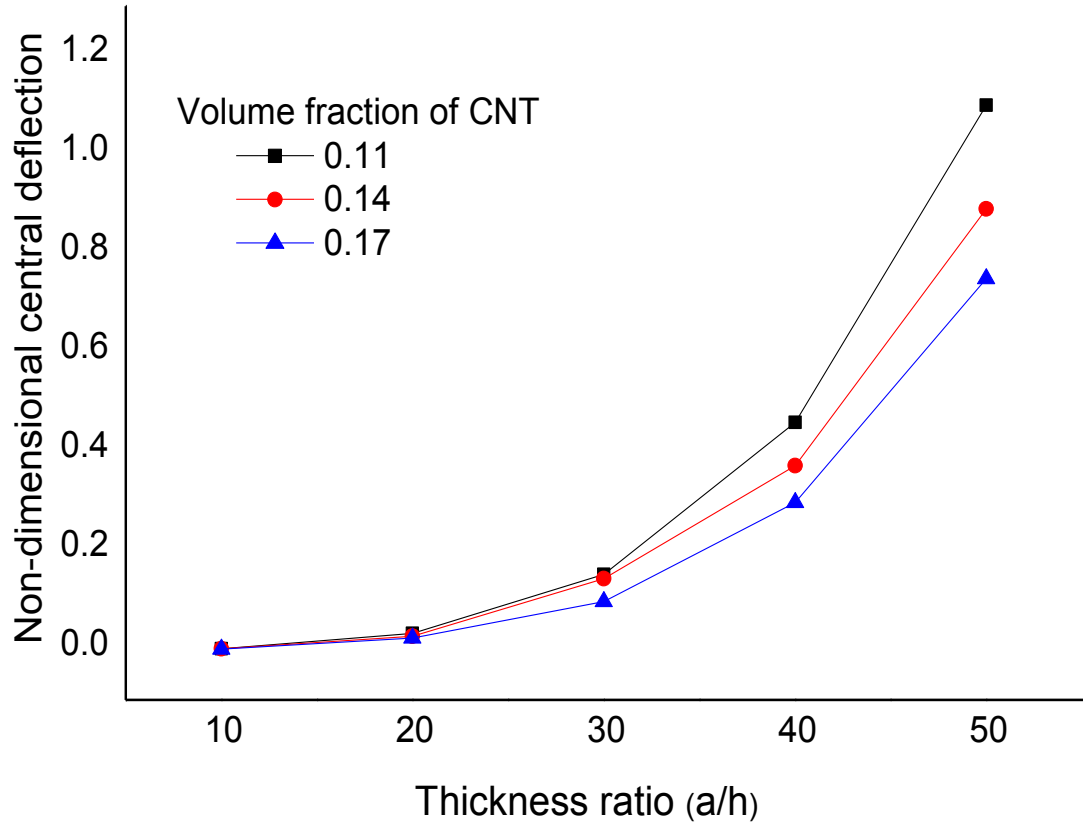


Fig.13: Effect of thickness ratio on non-dimensional central deflection.

4.3.2 Free vibration analysis.

In free vibration analysis, the non-dimensional fundamental frequency is obtained using $\varpi = \omega(a^2/h)\sqrt{\rho^m/E^m}$. Where ω is the natural frequency. The non-dimensional natural frequency of CNT composites square plates are subjected to same influence from thickness ratio and the volume fraction of CNT. Figs. 14-16 shows the effect of non-dimensional fundamental frequency of composite plate increasing with thickness ratio (a/h) and also increasing with the CNT volume fraction for different support condition (SSSS, CCCC and SCSC).

Table.7: The non-dimensional fundamental frequency for different thickness ratio (a/h) validation (SSSS).

a/h	Zhu et al.[1] ($V_{CNT}=0.11$)	Present	Zhu et al.[1] ($V_{CNT}=0.14$)	Present	Zhu et al.[1] ($V_{CNT}=0.17$)	Present
10	13.532	13.52938	14.306	14.31735	16.815	16.80776
20	17.352	17.33785	18.921	18.9309	21.456	21.43006
30	18.512	18.49868	20.415	20.43362	22.841	22.8248
40	18.973	18.96625	21.05	21.05459	22.402	22.385
50	19.223	19.19585	21.354	21.36252	23.697	23.6575

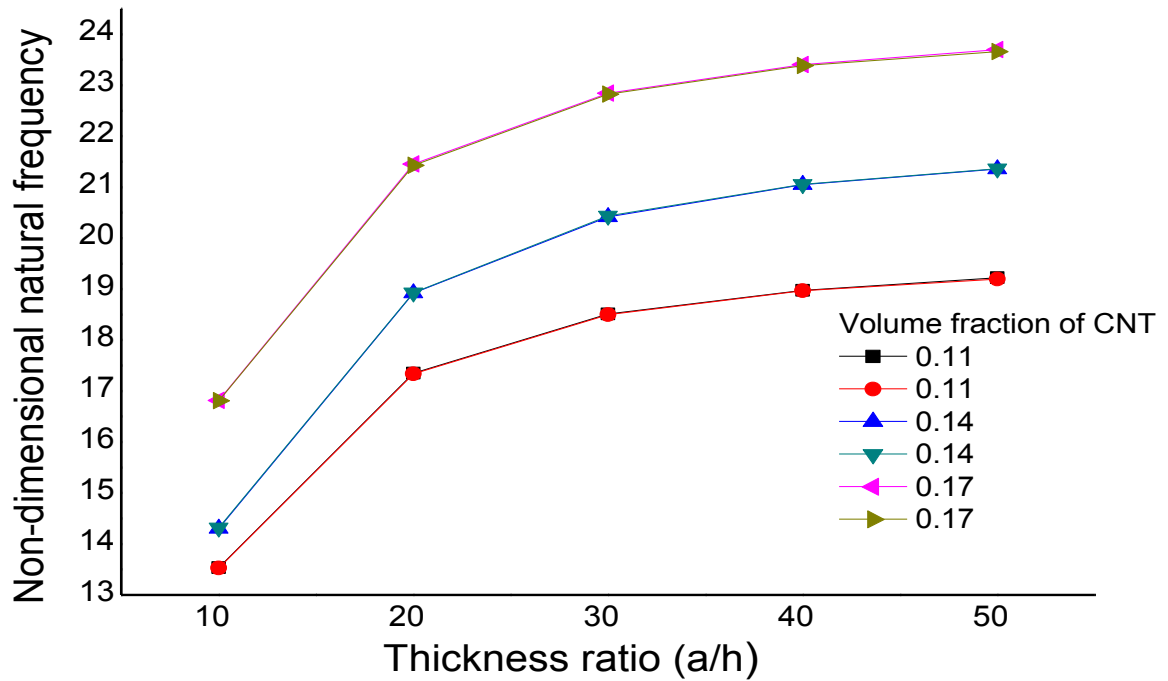


Fig.14: The effect of thickness ratio on non-dimensional fundamental frequency.

Table.8: The non-dimensional fundamental frequency for different thickness ratio (a/h).

(a) CCCC.

a/h	($V_{CNT} = 0.11$)	($V_{CNT}=0.14$)	($V_{CNT}=0.17$)
10	17.63852	18.14926	22.02397
20	28.39914	29.93935	35.30868
30	34.44871	37.05178	42.68662
40	37.76281	41.15209	46.6952
50	39.6704	43.5893	48.9897

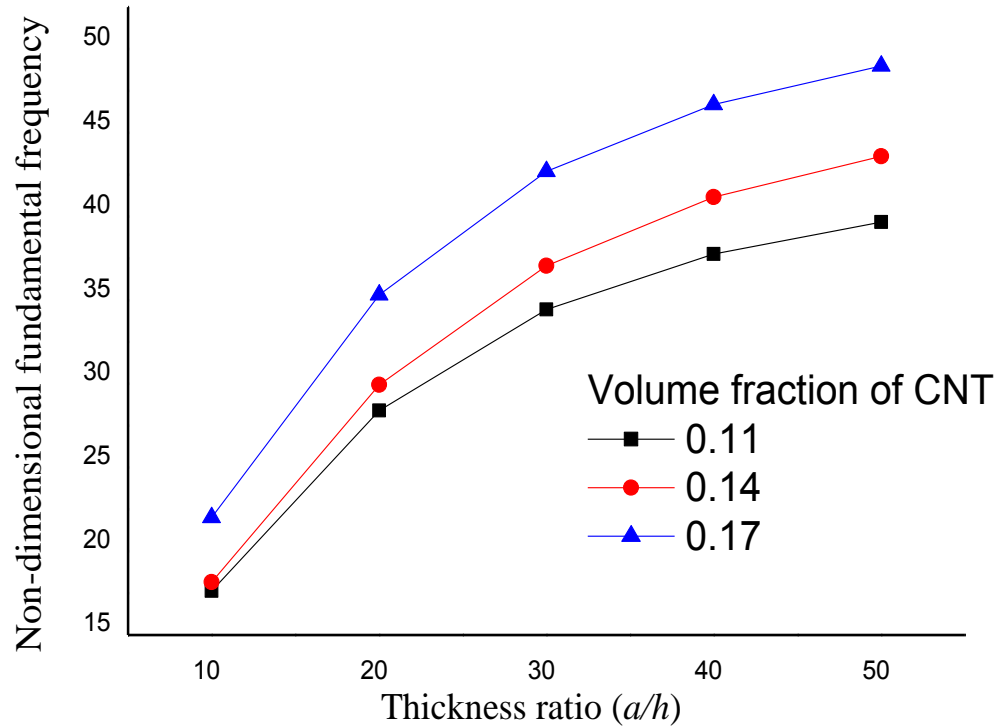


Fig.15: The effect of thickness ratio on non-dimensional fundamental frequency.

Table.9: The non-dimensional fundamental frequency for different thickness ratio (a/h).

(a) SCSC

a/h	($V_{CNT}=0.11$)	($V_{CNT}=0.14$)	($V_{CNT}=0.17$)
10	14.60667	15.37324	18.16507
20	18.34593	19.88725	22.70606
30	19.4875	21.36131	24.07742
40	19.94716	21.9715	24.62844
50	20.17313	22.27352	24.8972

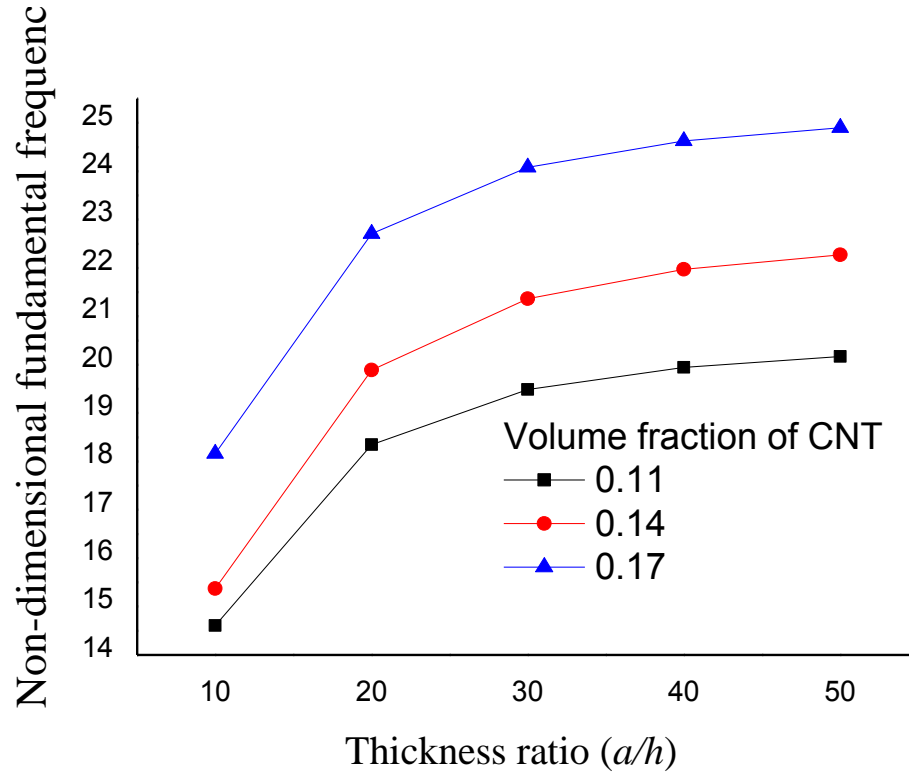


Fig.16: The effect of thickness ratio on non-dimensional fundamental frequency.

CHAPTER 5

CONCLUSION

Free vibration and bending behaviour of uniformly distributed carbon nanotube composite plate is analysed. The material properties of single-walled carbon nanotube evaluated through molecular dynamics simulation using LAMMPS software. The effective material properties of the composite plates are obtained using an extended rule of mixture. A finite element model is developed for the single-walled carbon nanotube composite plate using ANSYS Parametric Design Language (APDL) code in ANSYS environment. For the discretization purpose, an eight-noded serendipity shell element is used from the ANSYS library. Subsequently, the validation study is performed through the available published literature. Finally, the parametric study is demonstrated by varying different material and geometrical parameters for free vibration and bending responses of composite plate. The present idea is validated through the judgment with those available in the literature paper. Some new analytical investigation for different volume fractions, boundary conditions, and temperature are explained. Based on the present study over the free vibration and bending analysis performance of SWCNT composite plate, some arguments are concluded.

Based on the above statistical analysis the following conclusions are made:

- The non-dimensional elastic modulus longitudinal parameter with increase in CNT volume fractions.
- Free vibration is observed that the non-dimensional fundamental frequency is increasing with the volume fraction of CNT and also increasing the thickness ratio.
- The non-dimensional central deflections are increasing with the thickness ratios and the volume fractions.

Future Scope of the Research

- Bending analysis of functionally graded carbon nanotubes composites plates can be performed.
- Free vibration of functionally graded multi-walled carbon nanotubes composites (MWCNT) plates can be performed.
- The effective material properties of CNT based on composite material will be estimated through different material technique such as represented volume element (RVE), Mori-Tanaka approach etc.

.

REFERENCES

- [1] Zhu, P., Lei, Z. X. and Liew, K. M. (2012), “Static and free vibration analyses of carbon nanotube-reinforced composite plates using finite element method with first order shear deformation plate theory” composite structure, vol. 94, pp. 1450-1460.
- [2] Han, Y. and Elliott, J. (2007), “Molecular dynamics simulations of the elastic properties of polymer/carbon nanotube composites” comput. Materials sci., vol. 39, pp. 315-323.
- [3] Jin, Y. and Yuan, F.G. (2003), “Simulation of elastic properties of single-walled carbon nanotubes” Comput. Material sci., vol. 63, pp. 1507–1515.
- [4] Kumar, P. and Srinivas, J. (2014), “Numerical evaluation of effective elastic properties of CNT-reinforced polymers for interphase effects” Comput. Materials sci., vol. 88, pp.139-144.
- [5] Rossi, M. and Meo, M. (2009), “Estimation of mechanical properties of single-walled carbon nanotubes by using a molecular-mechanics based FE approach,” composites sci. and tech., vol. 69, pp. 1394-1398.
- [6] Alibeigloo, A. and Liew, K. M. (2013), “Thermoelastic analysis of functionally graded carbon nanotube-reinforced composite plate using theory of elasticity” composite structure, vol. 106, pp. 873-881.
- [7] Ansari, R., Rouhi, S. Aryayi, M. and Mirnezhad, M. (2012), “On the buckling behaviour of single-walled silicon carbide nanotubes” scientia iranica, vol. 19, pp. 1984-1990.
- [8] Murmu, T. and Pradhan, S. C. (2009), “Buckling analysis of a single-walled carbon nanotube embedded in an elastic medium based on nonlocal elasticity and Timoshenko beam theory and using DQM” Physica, E., vol. 41, pp. 1232-1239.
- [9] Shen, H. S. (2009), “Nonlinear bending of functionally graded carbon nanotube-reinforced composite plates in thermal environments” composite structure, vol. 91, pp. 9-19.
- [10] Popov, V. N., Doren, V. E. V. and Balkanski, M. (2000), “Elastic properties or critical of single-walled carbon nanotubes” solid state communications, vol. 114, pp. 395-399.

- [11] Ayatollahi, M. R., Shadlou, S. and Shokrieh M. M. (2011), “Multiscale modelling for mechanical properties of carbon nanotube reinforced nanocomposites subjected to different type of loading” composite structure, vol. 93, pp. 2250-2259.
- [12] Odegard, G. M., Gates, T. S., Wise, K. E., Park, C. and Siochi, E. J. (2003), “constitutive modelling of nanotube-reinforced polymer composites” composite sci. and tech., vol. 63, pp. 1671-1687.
- [13] Shen, H. S. and Xiang, Y. (2013), “Postbuckling of nanotube-reinforced composite cylindrical shells under combined axial and radial mechanical loads in thermal environment” composite part B, vol. 52, pp. 311-322.
- [14] Thai, H. T. (2012), “A nonlocal beam theory for bending buckling and vibration of nanobeams” Inter. Journal of engg. Sci., vol.52, pp. 56-64.
- [15] Chen, X. L., and Liu, Y. J. (2004), “Square representative volume element for evaluating the effective material properties of carbon nanotube-based composites” computational material science, vol. 29. PP. 1-11.
- [16] Guo, X., Leung, A. Y. T., He, X.Q., Jiang, H. and Huang, Y. (2008), “Bending buckling of single-walled carbon nanotubes by atomic-scale finite element” Composite part B, vol. 39, pp. 202-208.
- [17] Zhang, D., Rangarajan, A. and Wass, A. M., “Compressive behaviour and buckling response of carbon nanotubes” College of engineering, University of Michigan, Ann Arbor, MI-48109,USA.
- [18] Mohammadimehr, M., Saldi, A. R., Arani, A. G., Arefmanesh, A. and Hal, Q. (2010), “Buckling analysis of double-walled carbon nanotubes embedded in an elastic medium under axial compression using non-local Timoshenko beam theory” Manuscript.
- [19] Sears, A. and Batra, R.C. (2006), “Buckling of multiwalled carbon nanotubes under axial compression” Physical review B, vol. 73, pp. 085410-11.

- [20] Vodenitcharova, T. and Zhang, L. C. (2006), "Bending and local buckling of a nanocomposite beam reinforced by a single-walled carbon nanotube" *Inter. National jour. of solid and structure*, vol. 43, pp. 3006-3024.
- [21] Sun, Y. and Liew, K. M. (2008), "The buckling of single-walled carbon nanotubes upon bending: The higher order gradient continuum and mesh-free method" *Comput. Method Appl. Mech. Engg.*, vol. 197, pp. 3001-3013.
- [22] Yan, J. W., Liew, K. M. and He, L. H. (2012), "Analysis of single-walled carbon nanotubes using the moving kriging interpolation" *Comput. Method Appl. Mech. Engrg.*, vol. 229-232, pp. 56-67.
- [23] Giannopoulos, G. I., Kakavas, P. A. and Anifantis, N. K. (2008), "Evaluation of the effective mechanical properties of single walled carbon nanotubes using a spring based finite element approach" *Comput. materials sci.*, vol. 41, pp. 561-569.
- [24] Lei, Z. X., Liew, K. M. and Yu, J. L. (2013), "Free vibration analysis of functionally graded carbon nanotube-reinforced composite plates using the element-free kp-Ritz method in thermal environment" *Composite structure*, vol. 106, pp. 128-138.
- [25] Aydogdu, M. (2009), "A general nonlocal beam theory: Its application to nanobeam bending, buckling and vibration" *Physica E*, vol. 41, pp. 1651-1655.
- [26] Simsek, M. (2010), "Vibration analysis of a single-walled carbon nanotube under action of a moving harmonic load based on nonlocal elasticity theory.
- [27] Fiedler, B., Gojny, F. H., Wichmann, M. H. G., Nolte, M. C. M. and Schulte, K. (2006), "Fundamental aspects of nano-reinforced composites" *composites sci. and tech.*, vol. 66, pp. 3115-3125.

- [28] Lu, X. and Hu, Z. (2012), “Mechanical property evaluation of single-walled carbon nanotubes by finite element modelling” *Composite: Part B*, vol. 43, pp. 1902-1913.
- [29] Yu, H., Zhou, X., Zhang, W., Peng, H., Zhang, C. and Sun, K. (2011), “Properties of carbon nano-tubes-Cf/SiC composite by precursor infiltration and pyrolysis process” *Material and Design*, vol. 32, pp. 3516-3520.
- [30] Formica, G., Lacarbonara, W. and Alessi, R. (2010), “Vibration of carbon nanotube-reinforced composites” *Journal of sound and vibration*” vol. 329, pp. 1875-1889.
- [31] Volkov, A. N., Shiga, T., Nicholson, D., Shiomi, J. and Zhigilei, L. V. (2012), “Effect of buckling of carbon nanotubes on thermal conductivity of carbon nanotube material” *Journal of applied physics*, vol. 111, pp. 053501-11.
- [32] Odegard, G. M., Gates, T. S., Nicholson, L. M. and Wise, K. E. (2002), “Equivalent-Continuum modelling of nano-structured materials” *Composite science and tech.*, vol. 62, pp. 1869-1880.
- [33] Ma, P. C., Mo, S. Y., Tang, B. Z. and Kim, J. K. (2010), “Dispersion, interfacial interaction and re-agglomeration of functionalized carbon nanotubes in epoxy composites” *Carbon*, vol. 48, pp. 1824-1834.
- [34] Liu, Y. J. and Chen, X. L. (2003), “Evaluation of the effective material properties of carbon nanotube-based composite using a nanoscale representative volume element” *Mechanics of materials*, vol. 35, pp. 69-81.
- [35] Coleman, J.N., Khan, U., Blau, W.J., K.Y. and Gunko. (2006), “A review of the mechanical properties of carbon nanotube-polymer composites”, *Comput material sci.*, vol. 44, pp. 1624-1652.

[36] Kreupl, F., Graham, A. P., Liebau, M., Duesberg, G. S., Seidel, R. and Unger, E., “Carbon nanotubes for interconnect application” Infineon technologies AG, Corporate research, Otto-Hahn-Ring 6, 81739 Munich, Germany.

[37] Grace, T. (2013) “An introduction to carbon nanotubes” Center on polymer interface and macromolecular assemblies, pp. 1-14.

[38] Dresselhaus, MS. (1997), “Future directions in carbon science”, Annual Review of Material Science, vol. 27, pp.1–34.

[39] Cornwell, CF. and Wille, LT. (1997), “Elastic properties of single-walled carbon nanotubes in compression” Solid State Communications, vol. 101, pp.555–8.